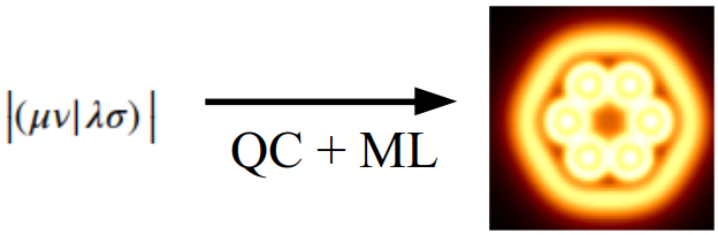
Quantum Chemistry and Artificial Intelligence
Master 2 internship - 2022

Context

Quantum chemistry (QC) is the application of quantum mechanics to compute the physicochemical properties of atomistic and molecular systems. There are various QC methods, which have been efficiently implemented in numerous packages [2]. A common bottleneck of these approaches is computing and handling an enormous number of two-electron integrals. Therefore, there is a continuous search for always faster methods to compute these integrals.



Internship description

The goal of the Master project is to rely on approximated QC models to predict these two-electron integrals for large molecular systems, which can be solved very efficiently, and to augment them with a data driven component. The integrals can be approximated with the Schwarz bound [3]: this model provides estimates of the complete set of integrals using only a small number of integrals that can be efficiently computed and stored. We will then adapt the method in [4] to complete this simplified model and correctly described the observations.

Such approach will speed-up the computations of these integrals by several orders of magnitude, opening unprecedented possibilities in QC. The student will implement the simplified model for sets of integrals that have already been computed using the Quantum Package code [1]. They will then adapt the method reported in [4] to complete the model.

Required skills

We are looking for a last year Master's or engineering degree student in applied mathematics, computer science, artificial intelligence or equivalent.
Knowledge of and experience in Python programming is a plus, and experience in deep learning frameworks (Tensorflow, Pytorch) is a must. The ideal candidate has a good knowledge of either artificial intelligence or Quantum chemistry.

Location and duration

This position is for a 5-months internship, with a flexible starting date in 2022. The internship will take place at Sorbonne University (4 Place Jussieu, 75005) and the Conservatoire National des Arts et Métiers (CNAM), situated in Paris (2, rue Conté, 75003). The internship will be co-supervised between the machine learning team (Vertigo) of the Center for Studies and Research in Computer Science and Communication (CEDRIC), and the Laboratoire de Chimie Physique-Matière et Rayonnement (LCPMR). The internship reward is 600 euros/month.

How to apply

Please send your application (CV and a short motivation letter) to
Nicolas.Sisourat@sorbonne-universite.fr and nicolas.thome@lecnam.net.

References

[1] Y. Garniron, T. Applencourt, K. Gasperich, A. Benali, A. Ferté, J. Paquier, B. Pradines, R. Assaraf, P. Reinhardt, J. Toulouse, P. Barbaresco, N. Renon, G. David, J.-P. Malrieu, M. Véril, M. Caffarel, P.-F. Loos, E. Giner, and A. Scemama. Quantum package 2.0: An open-source determinant-driven suite of programs. *Journal of Chemical Theory and Computation*, 15(6):3591–3609, 2019.

[2] C. D. Sherrill, D. E. Manolopoulos, T. J. Martínez, and A. Michaelides. Electronic structure software. *The Journal of Chemical Physics*, 153(7):070401, 2020.

[3] J. L. Whitten. Coulombic potential energy integrals and approximations. *The Journal of Chemical Physics*, 58(10):4496–4501, 1973.

[4] Y. Yin, V. L. Guen, J. Dona, E. de Bézenac, I. Ayed, N. Thome, and P. Gallinari. Augmenting physical models with deep networks for complex dynamics forecasting. *International Conference on Learning Representations*, 2021.